

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 14.8

Global applicability domain: Inside

Local applicability domain index: 5.20e-01

Confidence level: 5.31e-01

Nearest Neighbors from the Training Set

Image not found

Molinate

Measured: 25.7

Predicted: 14.8

Image not found

Butyl ether

Measured: 72.4

Predicted: 32.3

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Acetamide, N-methyl-N-phenyl-

Measured: 1.51

Predicted: 2.53

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Phenacetin

Measured: 30.2

Predicted: 3.76